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Width Anomaly in Resonant Tunneling Structures

by

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WIDTH ANOMALY IN RESONANT TUNNELING STRUCTURES

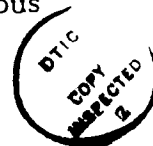
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We have found anomalous behavior in the variation of width and position of the resonance as a function of the effective mass Hamiltonian parameter. This is an addendum to our previous paper, Solid State Communications 72, 7 (1989).



A-1

Recently,¹ we analyzed a resonant tunneling structure (a single well formed by two barriers of finite widths and heights,² henceforth referred to as RTS) by using a general effective mass Hamiltonian,³ and found that physical properties such as dwell time and average speed depend considerably on the matching parameter. For the sake of completeness, the effective mass Hamiltonian and the physical properties of the RTS are described briefly here. The stationary-state properties of an RTS in the effective mass approximation are obtained by solving the Schrödinger equation for the envelop function $\Psi(x)$ along the growth direction x , where the mass also varies as x :

$$\left[-\frac{\hbar}{2}m^a(x)\frac{d}{dx}m^b(x)\frac{d}{dx}m^a(x) + V(x) - E\right]\Psi(x) = 0. \quad (1)$$

Here $V(x)$ is the RTS potential profile

$$V(x) = \begin{cases} V_1, & \text{if } 0 \leq x \leq a_1, \\ 0, & \text{if } a_1 \leq x \leq a_1 + d, \\ V_2, & \text{if } a_1 + d \leq x \leq a_1 + d + a_2, \end{cases}$$

where V_i and a_i ($i=1,2$) are the heights and widths of the barriers, d is the width of the well, $m(x)$ is the effective mass, and $2a + b = -1$ from the dimensionality condition with a and b as constants. These constants ensure that the Hamiltonian is Hermitian. The kinetic energy operator of Eq. (1) dictates that $m^a(x)\Psi(x)$ and $m^{a+b}(x)\frac{d\Psi(x)}{dx}$ must be continuous across the interface, implying the physical result that the current density $j \propto \Re\left\{\frac{\Psi^*}{m(x)}\frac{d\Psi}{dx}\right\} = \Re\{m^a(x)\Psi^*m^{a+b}(x)\frac{d\Psi}{dx}\}$ be continuous. However, in general, the charge density $\rho \propto \Psi^*\Psi$ need not be continuous across an interface. For the special case of $a = 0$ and $b = -1$ one obtains, in addition, the continuity of charge density. So, this is a single-parameter b ($a = -\frac{1+b}{2}$) problem.

The resonance states depend on b , as demonstrated in our earlier paper,¹ where we concluded that one can not *a priori* prefer one value of b over another. It was also suggested that to better understand the underlying physics and also to fix a value of b , one needs to do some microscopic calculations.

The study of Ref. 1 was mainly concentrated on the calculation of the dwell time τ_D over the region 0 to x_1 of the structure, with x_1 extending from 0 to $a_1 + d + a_2$,

defined^{1,4} as the integrated probability density of the electron per unit incidence flux

$$\tau_D(x) = \int_0^x dy \frac{m(y)}{\hbar k} |\Psi(y)|^2, \quad (2)$$

where $k = \sqrt{\frac{2m(y)E}{\hbar^2}}$, and a constant value for $m(y)$ (0.067) has been assumed in Eq.(2) to calculate $\tau_D(x)$. The associated average local speed was also calculated, and in the variation of local speed as a function of x , there were discontinuities observed at the interfaces.

The values of the resonance energy and the energy at half of the maximum transmission for a symmetric RTS and the resonance energy for an asymmetric RTS for given values of b were displayed in Table 1 of Ref. 1, which indirectly shows the variation of the width of the first resonance state as a function of b . In this addendum, we have studied in particular the parameter b dependence of the position and width of the first three resonance states of a RTS. The variation of $\tau_D(x)$ as a function of x for different values of b is also shown.

A slightly different RTS than the one studied in the Ref. 1 is under investigation here² since the RTS of Ref. 1 does not have three resonance states (the reason to choose the RTS with three resonance states is pointed out later in the text). Figure 1 displays the first resonance energy E_R in panel (1) and width ΔE_R in panel (2) as functions of the parameter b . Panel (3) displays τ_D as a function of x for three different b values, -2, 0 & 2. The change in b from -2 to 2 moves the first resonance state considerably up, whereas its width, panel (2), decrease as b increases from -2 to 2. This variation of width is also clear from the plot of τ_D versus x , where a broader resonance implies less average time spent by an electron in the RTS and vice versa. Even though $\tau_D(x)$, the average time spent by an electron inside the RTS, depends strongly on b , $\Delta E_R \tau_D(a_1 + d + a_2)$ has been found independent of b and approximately equal to $2\hbar$, which is twice the escape time τ_{esc} ($\Delta E_R \tau_{esc} \sim \hbar$) of the electron from the resonance state.

The variation of the position and width was further analyzed for the second resonance state of the RTS of Ref. 1 (which only has two resonances) in order to assess the general pattern. Results of this investigation

are not shown here for the brevity. It was found that by changing b from -2 to 2, the width of the second resonance state increases as the resonance energy increases, in contrast to what has been found for the first resonance state. A very simple explanation for such behavior could have been that the wavefunction of the first resonance state is symmetric whereas the wavefunction of the second one is asymmetric, and one would expect two different wavefunctions to respond differently to a change in b . We should mention here that the width of the first resonance state always decreases as b increases for an RTS with either two or three resonance states, and Fig. 1 shows the results for the RTS of Ref. 2 with three resonance states.

To make sure that it is the nature of the wavefunction of the resonance state which causes the anomaly in the variation of the widths of different resonance states, one should study a system which at least has two resonance states with the same kind of wavefunction. This is the reason to consider a different RTS than the one studied in Ref. 1. Figure 2 shows the results for the second resonance state of the RTS of Ref. 2. The resonance energy increases, whereas the width of the resonance goes through a maximum as the parameter b increases. This maximum in the plot of the width versus b is also apparent in the variation of $\tau_D(x)$ as a function of x (panel 3 of Fig. 2), where the average time spent by an electron is almost the same for the -2 and 0 values of b . It would be wise to note here that for the second resonance state we also have $\Delta E_{RTD}(a_1 + d + a_2) \sim 2\hbar$. Figure 3 displays the results for the third resonance state, where the variation of E_R and ΔE_R as b in panel (1) and (2), respectively, and $\tau_D(x)$ as x in panel (3) are the same as those found for the second resonance state of the RTS of Ref. 1. The equality $\Delta E_{RTD}(a_1 + d + a_2) \sim 2\hbar$ is also true for this resonance state.

Most of the experimental observations are analyzed with the model calculations based on several approximations and presumptions, and as far as the literature goes, we do not think that a definite boundary condition for such an abrupt interfaces has yet been found. It has always been presumed that $b = -1$ and $a = 0$. Unless there is an exact theoretical investigation to establish a boundary condition for such a system, the boundary condition will remain as that one of parameter fitting to

the experimental data. In conclusion, since the anomalous variation of the widths of the resonance states can not be attributed to the nature of the wavefunctions of these states, a microscopic calculation^{5,6} of such a system could resolve this problem. A further investigation in order to find a boundary condition is under way to study the effect of b on the position of impurity levels in quantum confined structures.

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Figure Captions

- Fig. 1. Resonance energy E_R (panel 1) and width ΔE_R (panel 2) as functions of the parameter b . Panel 3 shows the dwell time τ_D as a function of position x . The physical parameters of the RTS studied are given in Ref. 2.
- Fig. 2. Same as in Fig. 1 but for the second resonance state.
- Fig. 3. Same as in Fig. 1 but for the third resonance state.

Fig. 1

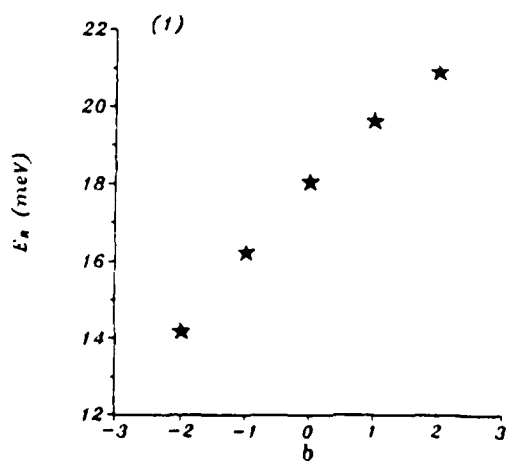
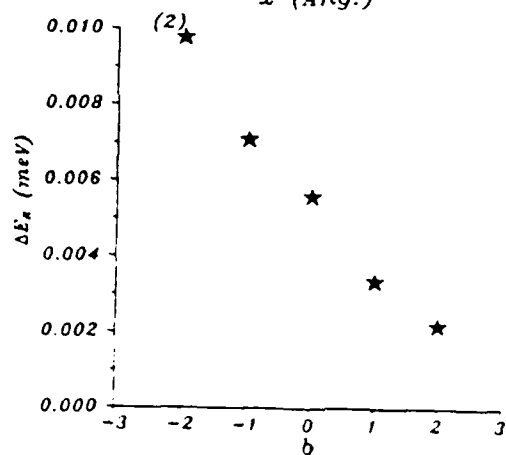
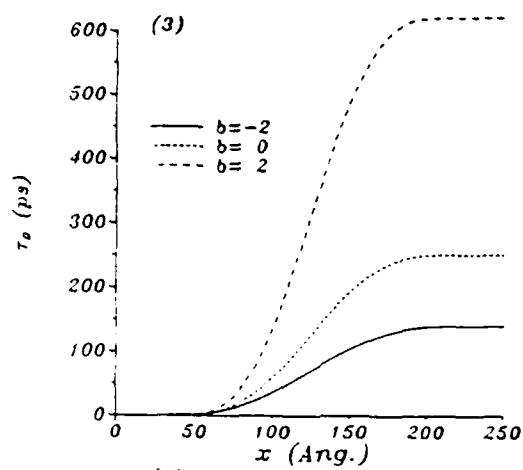


Fig. 2

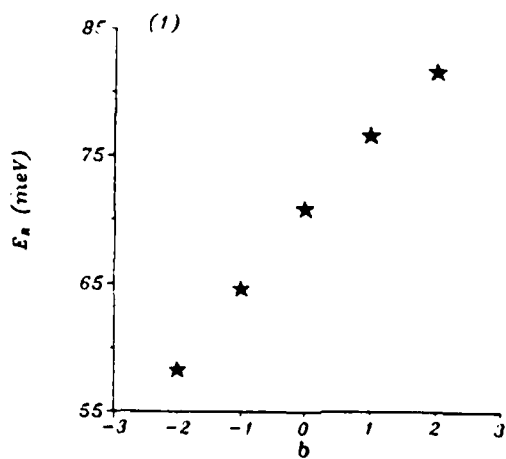
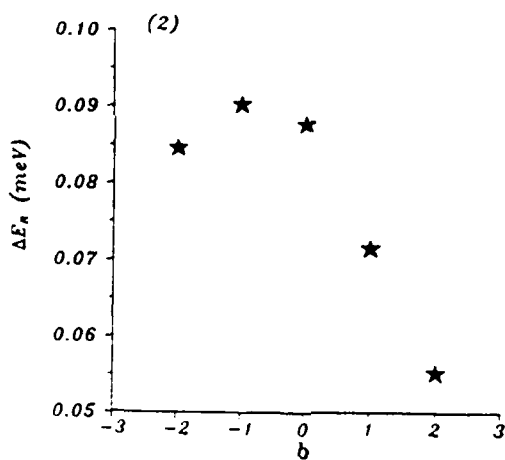
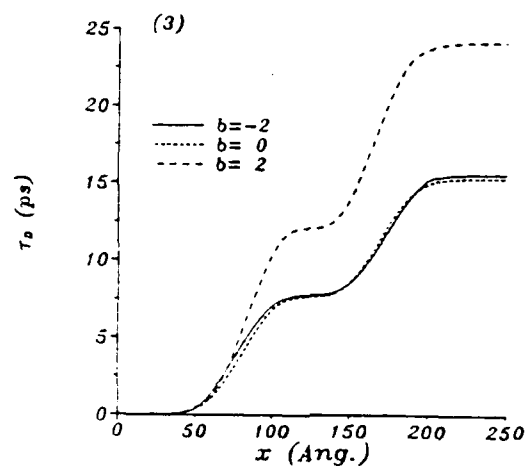


Fig. 3

